

Ethyl lactate
97-64-3 | DTXSID6029127

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.05 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.80e-01

Confidence level: 5.44e-01

Nearest Neighbors from the Training Set

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Ethyl isobutyrate

Measured: 3.75

Predicted: 19.3

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Phenyl phosphorodichloridate

Measured: 5.23e-02

Predicted: 1.16e-02

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2-Butanone, 1-bromo-

Measured: 1.26e-01

Predicted: 7.89

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Ethyl chloroacetate

Measured: 9.05e-01

Predicted: 7.43